



chain nodes :

7 8 9 16 17 18 20 21 28 29 30 31 45 46 47 48 49

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15 22 23 24 25 26 27 32 33 34 35 36 37 39
40 41 42 43 44

chain bonds :

5-7 6-16 7-8 7-9 9-12 16-17 17-18 18-20 18-21 26-29 27-28 29-30 29-31 31-33 39-46
44-45 47-48 47-49

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15 22-23 22-27 23-24
24-25 25-26 26-27 32-33 32-37 33-34 34-35 35-36 36-37 39-40 39-44 40-41 41-42
42-43 43-44

exact/norm bonds :

6-16 7-8 7-9 9-12 17-18 18-20 18-21 27-28 29-30 29-31 31-33 39-46 44-45 47-48

exact bonds :

5-7 16-17 26-29 47-49

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15 22-23 22-27 23-24
24-25 25-26 26-27 32-33 32-37 33-34 34-35 35-36 36-37 39-40 39-44 40-41 41-42
42-43 43-44

isolated ring systems :

containing 1 : 10 : 22 : 32 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:Atom 20:CLASS 21:CLASS 22:Atom
23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:Atom
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom
44:Atom 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:Atom

Generic attributes :

18:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : Exactly 1

Type of Ring System : Monocyclic

fragments assigned reactant role:

containing 22

containing 39

fragments assigned product role:

containing 1

Element Count :

Node 18: Limited

N,N1

C,C5